Topological insulators with quaternionic analytic Landau levels

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We study the 3D topological insulators in the continuum by coupling spin-$\frac{1}{2}$ fermions to the Aharonov-Casher $SU(2)$ gauge field. They exhibit flat Landau levels in which orbital angular momentum and spin are coupled with a fixed helicity. Each Landau level contributes one branch of gapless helical Dirac modes to the surface spectra, whose topological properties belong to the $\mathbb{Z}_2$-class. The lowest Landau level states exhibit the quaternionic analyticity as a generalization of the complex analyticity of the 2D case. The flat Landau levels can be generalized to an arbitrary dimension. Interaction effects and possible experimental realizations are also discussed.

The 2D quantum Hall (QH) systems [1, 2] are among the earliest examples of quantum states characterized by topology [3, 4] rather than symmetry in condensed matter physics. Their magnetic band structures possess topological Chern numbers defined in time-reversal (TR) symmetry breaking systems [3, 5]. The consequential quantized charge transport originates from chiral edge modes [6, 7], a result from the chirality of Landau level wavefunctions. Current studies of TR invariant topological insulators (TIs) have made great success in both 2D and 3D. They are described by a $\mathbb{Z}_2$-invariant which is topologically stable with respect to TR invariant perturbations [8–17]. On open boundaries, they exhibit odd numbers of gapless helical edge modes in 2D systems and surface Dirac modes in 3D systems. TIs have been experimentally observed through transport experiments [18–20] and spectroscopic measurements [21–27].

The current research of 3D TIs has been focusing on the Bloch-wave band structures. Nevertheless, LLs possess the advantages of the elegant analytic properties and flat spectra, both of which have played essential roles in the study of 2D integer and fractional QH effects [28–36]. As pioneered by Zhang and Hu [37], LLs and QH effects have been generalized to various high dimensional manifolds [37–42]. However, to our knowledge, TR invariant LLs have not been studied in 3D flat space before. It would be interesting to develop the LL counterpart of 3D TIs in the continuum independent of the band inversion mechanism. The analytic properties of 3D LL wavefunctions and the flatness of their spectra provide an opportunity for further investigation on non-trivial interaction effects in 3D topological states.

In this article, we propose flat LLs in 3D space in which spin-$\frac{1}{2}$ fermions are coupled to an isotropic $SU(2)$ Aharonov-Casher potential. When odd number LLs are fully filled, the system is a 3D $\mathbb{Z}_2$ TI with TR symmetry. Each LL state has the same helicity structure, *i.e.*, the relative orientation between orbital angular momentum and spin. Just like that the 2D lowest LL (LLL) wavefunctions in the symmetric gauge are complex analytic functions, the 3D LLL ones are mapped into quaternionic analytic functions. Different from the 2D case, there is no

magnetic translational symmetry for the 3D LL Hamiltonian due to the non-Abelian nature of the gauge field. Nevertheless, magnetic translations can be applied for the Gaussian pocket-like localized eigenstates in the LLL. The edge spectra exhibit gapless Dirac modes. Their stability against TR invariant perturbations indicates the $\mathbb{Z}_2$ nature. This scheme can be easily generalize to N dimensions. Interaction effects and the Laughlin-like wavefunctions for the 4D case are constructed. Possible realizations of the 3D LL system are discussed.

We begin with the 3D LL Hamiltonian for a spin-$\frac{1}{2}$ non-relativistic particle as

$$H^{3D,LL} = \frac{1}{2m}\sum_a \left\{ -i\hbar\nabla^a - \frac{q}{c}A^a(\vec{r}) \right\}^2 + V(r), \quad (1)$$

where $A^a_{\alpha\beta} = \frac{1}{2}G\epsilon_{abc}\sigma^b_{\alpha\beta}r^c$ is a 3D isotropic $SU(2)$ gauge with Latin indices run over x, y, z and Greek indices denote spin components $\uparrow, \downarrow$; G is a coupling constant and σ's are Pauli matrices; $V(r) = -\frac{1}{2}m\omega_0^2 r^2$ is a harmonic potential with $\omega_0 = |qG|/(2mc)$ to maintain the flatness of LLs. $\vec{A}$ can be viewed as an Aharonov-Casher potential associated with a radial electric field linearly increasing with r as $\vec{E}(r) \times \vec{\sigma}$. $H^{3D,LL}$ preserves the TR symmetry in contrast to the 2DQH with TR symmetry broken. It also gives a 3D non-Abelian generalization of the 2D quantum spin Hall Hamiltonian based on Landau levels studied in Ref. [8]. To see the 3D LL structure more explicitly, $H^{3D,LL}$ can be further expanded as a harmonic oscillator with a constant spin-orbit (SO) coupling as $H_{\mp} = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 r^2 \mp \omega_0 \vec{\sigma}\cdot\vec{L}$ where $\mp$ apply to the cases of $qG > 0$ (< 0), respectively. The spectra of Eq. 1 in the form of $H_{\mp}$ were studied in the context of the supersymmetric quantum mechanics [43]. However, its connection with Landau levels was not noticed. Eq. 1 has also been proposed to describe the electrodynamic properties of superconductors [44–46].

The spectra and eigenstates of Eq. 1 are explained as follows. We introduce the helicity number for the eigenstate of $\vec{L} \cdot \vec{\sigma}$, defined as the sign of its eigenvalue of the total angular momentum $\vec{J} = \vec{L} + \vec{S}$, which equals ± 1 for the sectors of $j_\pm = l \pm \frac{1}{2}$, re-
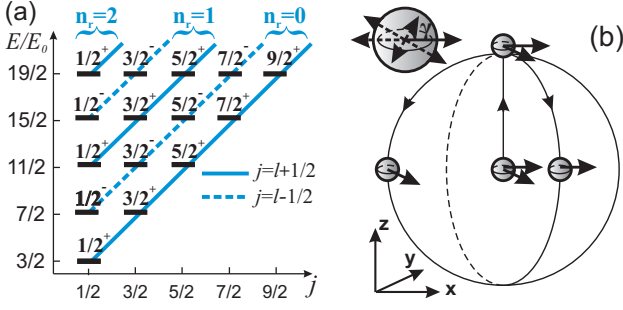
FIG. 1: a) The eigenstates of the 3D harmonic oscillator labeled by total angular momentum $j_\pm = l \pm \frac{1}{2}$. Following the solid diagonal (dashed) lines, these states are reorganized into the 3D LL sates with the positive (negative) helicity. b) The magnetic translation for the LLL state ($l = 0$) localized at the origin in the case of $qG > 0$, whose spin is set along an arbitrary direction in the xy-plane. The displacement vector $\vec{\delta}$ lies in the plane perpendicular to spin orientation. The resultant state remains in the LLL as a localized Gaussian pocket.

spectively. At $qG > 0$, the eigenstates are denoted as $\psi_{n_r;j_\pm,j_z;l}(\vec{r}) = R_{n_r,l}(r)\mathcal{Y}_{j_\pm,j_z;l}(\hat{\Omega})$, where the radial function is $R_{n_r l}(r) = r^l e^{-\frac{r^2}{4l_G^2}} F(-n_r, l + \frac{3}{2}, \frac{r^2}{2l_G^2})$; F is the confluent hypergeometric function and $l_G = \sqrt{\frac{\hbar c}{qG}}$ is the "magnetic" length; $\mathcal{Y}_{j_\pm,j_z;l}(\hat{\Omega})$ are angular solutions with $j_\pm = l \pm \frac{1}{2}$, respectively. Flat spectra appear with infinite degeneracy in the sector of j_+, where the energy dispersion $E_{n_r,l}^+ = (2n_r + \frac{3}{2})\hbar\omega_0$ is independent of l, and thus n_r serves as the LL index. For the sector of j_-, the energy disperses with l as $E_{n_r,l}^- = [2(n_r + l) + \frac{5}{2}]\hbar\omega_0$. Similar results apply to the case of $qG < 0$, where the infinite degeneracy occurs in the sector of j_-. These LL wavefunctions are the same as those of the 3D harmonic oscillator but with different organizations. As illustrated in Fig. 1 (a), these eigenstates along each diagonal line with the positive (negative) helicity fall into the flat LL states for the case of $qG > 0$ (< 0), respectively.

Compared to the 2D case, a marked difference is that the 3D LL Hamiltonian has no magnetic translational symmetry. The non-Abelian field strength grows quadratically with r as $F_{ij}(\vec{r}) = \partial_i A_j - \partial_j A_i - \frac{iq}{\hbar c}[A_i, A_j] = g\epsilon_{ijk}\{\sigma^k + \frac{1}{4l_G^2}r^k(\vec{\sigma} \cdot \vec{r})\}$. Nevertheless, magnetic translations still apply to the highest weight states of the total angular momentum $\vec{J} = \vec{L} + \vec{S}$ in the LLL at $qG > 0$. For simplicity, we drop the normalization factors of wavefunctions below. For the positive helicity states with $j_z = j_+$, $\vec{L}$ and $\vec{S}$ are parallel to each other. Their wavefunctions are denoted by $\psi_{\hat{z},l}^{hw}(\vec{r}) = (x + iy)^l e^{-\frac{r^2}{4l_G^2}} \otimes \alpha_{\hat{\Omega}=\hat{z}}$, where $\alpha_{\hat{\Omega}}$ is the spin eigenstate of $\hat{\Omega} \cdot \vec{\sigma}$ with eigenvalue 1. For these states, the magnetic translation is defined as usual $T_{\hat{z}}(\vec{\delta}) = \exp[-\vec{\delta} \cdot \vec{\nabla} + \frac{i}{4l_G^2}\vec{r}_{xy} \cdot (\hat{z} \times \vec{\delta})]$, where $\vec{\delta}$ is the displacement vector in the xy-plane and

$\vec{r}_{xy}$ is the projection of $\vec{r}$ in the xy-plane. The resultant state, $T_{\hat{z}}(\vec{\delta})\psi_{\hat{z},l}^{hw}(\vec{r}) = e^{i\frac{\vec{r}_{xy} \cdot (\hat{z} \times \delta)}{4l_G^2}} \psi_{\hat{z},l}^{hw}(\vec{r} - \vec{\delta})$, remains in the LLL. Generally speaking, the highest weight states can be defined in a plane spanned by two orthogonal unit vectors $\hat{e}_{1,2}$ as $\psi_{\hat{e}_3,l}^{hw}(\vec{r}) = [(\hat{e}_1 + i\hat{e}_2) \cdot \vec{r}]^l e^{-\frac{r^2}{4l_G^2}} \otimes \alpha_{\hat{e}_3}$ with $\hat{e}_3 = \hat{e}_1 \times \hat{e}_2$. The magnetic translation for such states is defined as $T_{\hat{e}_3}(\vec{\delta}) = \exp[-\vec{\delta} \cdot \vec{\nabla} + \frac{i}{4l_G^2} \vec{r}_{12} \cdot (\hat{e}_3 \times \vec{\delta})]$, where $\vec{\delta}$ lies in the $\hat{e}_{1,2}$-plane and $\vec{r}_{12} = \vec{r} - \hat{e}_3(\vec{r} \cdot \hat{e}_3)$. However, for other LLL states with $j_z \neq \pm j$ at $qG > 0$ and all the LLL states at $qG < 0$, their spin and orbit angular momenta are entangled. The above definition of magnetic translation fails. As an example, let us translate the LLL state localized at the origin as illustrated in Fig. 1 (b). We set the spin direction of $\psi_{\hat{e}_3,l=0}^{LLL}$ in the xy-plane parameterized by $\hat{e}_3(\gamma) = \hat{x}\cos\gamma + \hat{y}\sin\gamma$, i.e., $\alpha_{\hat{e}_3}(\gamma) = \frac{1}{\sqrt{2}}(|\uparrow\rangle + e^{i\gamma}|\downarrow\rangle)$, and translate it along $\hat{e}_1 = \hat{z}$ at the distance R. The resultant states read as $\psi_{\gamma,R}(\rho,\phi,z) = e^{i\frac{q}{2}R\rho\sin(\phi-\gamma)}e^{-|\vec{r}-R\hat{z}|^2/4l_G^2} \otimes \alpha_{\hat{e}_3}(\gamma)$, where $\rho = \sqrt{x^2 + y^2}$ and ϕ is the azimuthal angular of $\vec{r}$ in the xy-plane. Such a state remains in the LLL as an off-centered Gaussian wave packet.

The highest weight states and their descendent states from magnetic translations defined above have clear classic pictures. The classic equations of motion are derived as

$$\dot{\vec{r}} = \frac{1}{m}\vec{p} + 2\omega_0(\vec{r} \times \frac{1}{\hbar}\vec{S}), \quad \dot{\vec{p}} = 2\omega_0\vec{p} \times \frac{1}{\hbar}\vec{S} - m\omega_0^2\vec{r},$$
$$\dot{\vec{S}} = \frac{2\omega_0}{\hbar}\vec{S} \times \vec{L}, \tag{2}$$

where $\vec{p}$ is the canonical momentum, $\vec{L} = \vec{r} \times \vec{p}$ is the canonical orbital angular momentum, and $\vec{S}$ here is the expectation value of $\frac{\hbar}{2}\vec{\sigma}$. The first two describe the motion in a non-inertial frame subject to the angular velocity $\frac{2\omega_0}{\hbar}\vec{S}$, and the third equation is the Larmor precession. $\vec{L} \cdot \vec{S}$ is a constant of motion of Eq. 2. In the case of $\vec{S} \parallel \vec{L}$, we can prove that both $\vec{S}$ and $\vec{L}$ are conserved. Then the cyclotron motions become coplanar within the equatorial plane perpendicular to $\vec{S}$. Centers of the circular orbits can be located at any points in the plane.

The above off-centered LLL states break all the rotational symmetries. Nevertheless, we can recover the rotational symmetry around the axis from the origin to the packet center by performing the Fourier transform over $\psi_{\gamma,R}(\rho,\phi,z)$ with respect to the azimuthal angle γ of spin polarization. The resultant state is a j_z-eigenstate

$$\psi_{j_z=m+\frac{1}{2},R}(\rho,\phi,z) = \int_0^{2\pi} \frac{d\gamma}{2\pi}e^{im\gamma}\psi_{\gamma,R}$$
$$\propto e^{\frac{-|\vec{r}-R\hat{z}|^2}{4l_G^2}} e^{im\phi}\{J_m(x)|\uparrow\rangle + J_{m+1}(x)e^{i\phi}|\downarrow\rangle\}, \tag{3}$$

with $x = R\rho/(2l_G^2)$. In fact, $\psi_{\gamma,R}$'s are non-orthogonal to each other, thus this transformation is linear but not

unitary. For $R > 0$, although Eq. 3 exists for all the values of m, the norm of the direct result of this transformation decays as increasing $|m|$. At large distance of R, the spatial extension of $\psi_{j_z=m+\frac{1}{2},R}$ in the xy-plane is at the order of ml_G^2/R, which is suppressed at large values of R and scales linear with m. In particular, the narrowest states $\psi_{\pm\frac{1}{2},R}$ exhibit an ellipsoid shape with an aspect ratio decaying as l_G/R when R goes large. For those states with $|m| < R/l_G$, they localize within the distance of l_G from the center $R\hat{z}$. As a result, the real space local density of states of LLL grow linearly with R. In fact, this local density of state can be calculated exactly as $\rho(r) = \frac{1}{\pi l_G^3}\left\{\frac{1}{\sqrt{\pi}}e^{-\frac{r^2}{l_G^2}} + (\frac{r}{l_G} + \frac{l_G}{2r})\mathrm{erf}(\frac{r}{l_G})\right\}$, which approaches $\frac{r}{\pi l_G^4}$ as $r \to +\infty$.

In analogy to the fact that the 2D LLL states are complex analytic functions due to chirality, we have found an impressive result that the helicity in 3D LL systems leads to the quaternionic analyticity. Quaternion is the first discovered non-commutative division algebra, which has three anti-commuting imaginary units i, j and k, satisfying $i^2 = j^2 = k^2 = -1$ and $ij = k$. It has been applied in quantum systems [47, 48] and SO coupled BECs [49]. Just like two real numbers forming a complex number, a two-component complex spinor $\psi = (\psi_\uparrow, \psi_\downarrow)^T$ can be viewed as a quaternion defined as $f = \psi_\uparrow + j\psi_\downarrow$. In the quaternion representation, the TR transformation $i\sigma_2\psi^*$ becomes $Tf = -fj$ satisfying $T^2 = -1$; multiplying a U(1) phase factor $e^{i\phi}\psi$ corresponds to $fe^{i\phi}$; the SU(2) operations $e^{-i\frac{\sigma_x}{2}\phi}\psi$, $e^{-i\frac{\sigma_y}{2}\phi}\psi$, and $e^{-i\frac{\sigma_z}{2}\phi}\psi$ map to $e^{\frac{k}{2}\phi}f$, $e^{\frac{j}{2}\phi}f$, and $e^{-\frac{i}{2}\phi}f$, respectively. The quaternion version of $\psi_{j=j_+,j_z=m+\frac{1}{2}}^{LLL}$ is $f_{j_+,j_z}^{LLL}(x,y,z) = \Psi_{\uparrow,j_+,j_z} + j\Psi_{\downarrow,j_+,j_z}$, where $\Psi_{\uparrow,j_+,j_z} = \langle j_+,j_z|l,m;\frac{1}{2},\frac{1}{2}\rangle r^l Y_{l,m}$, $\Psi_{\downarrow,j_+,j_z} = \langle j_+,j_z|l,m+1;\frac{1}{2},-\frac{1}{2}\rangle r^l Y_{l,m+1}$. Please note that the Gaussian factor does not appear in f_{j_+,j_z}^{LLL} which is a quaternionic polynomial.

As a generalization of the Cauchy-Riemann condition, a quaternionic analytic function $f(x,y,z,u)$ satisfies the Fueter condition [50] as

$$\frac{\partial f}{\partial x} + i\frac{\partial f}{\partial y} + j\frac{\partial f}{\partial z} + k\frac{\partial f}{\partial u} = 0, \tag{4}$$

where x, y, z and u are coordinates in the 4D space. In Eq. 4, imaginary units are multiplied from the left, thus it is the left-analyticity condition which works in our convention. Below, we prove the LLL function $f_{j_+,j_z}^{LLL}(x,y,z)$ satisfying Eq. 4. Since f_{j_+,j_z}^{LLL} is defined in 3D space, it is a constant over u, and thus only the first three terms in Eq. 4 apply to it. Obviously the highest weight states with spin along the z-axis, $f_{j_+=j_z=l+\frac{1}{2}}^{LLL} = (x+iy)^l$, satisfy Eq. 4 which is reduced to complex analyticity. By applying an arbitrary SU(2) rotation g characterized by the Eulerian angles (α,β,γ), $f_{j_+=j_z}^{LLL}$ transforms to

$$f'^{,\,LLL}(x,y,z) = e^{-i\frac{\alpha}{2}}e^{j\frac{\beta}{2}}e^{-i\frac{\gamma}{2}}f_{j_+=j_z}^{LLL}(x',y',z'), \tag{5}$$

where (x',y',z') are the coordinates by applying the inverse of g on (x,y,z). We check that $(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y} + j\frac{\partial}{\partial z})f'^{LLL}(x,y,z) = e^{i\frac{\alpha}{2}}e^{-j\frac{\beta}{2}}e^{i\frac{\gamma}{2}}\left\{\frac{\partial}{\partial x'} + i\frac{\partial}{\partial y'} + j\frac{\partial}{\partial z'}\right\}f_{j_+,j_z}^{LLL}(x',y',z') = 0$. Essentially, we have proved that a quaternionic analytic function remains analytic under rotations. Since all the highest weight states are connected through SU(2) rotations, and they form overcomplete basis for the angular momentum representations, we conclude that all the 3D LLL states with the positive helicity are quaternionic analytic.

Next we prove that the set of quaternionic LLL states $f_{j_+=l+\frac{1}{2},j_z}^{LLL}$ ($j_+ \geq \frac{1}{2}, j_z \geq j_+ \geq -j_z$) form the complete basis for quaternionic valued analytic polynomials in 3D. We only need to prove it for each value of $j_+ = l + \frac{1}{2}$. Any linear superposition of the LLL states with j_+ can be represented as $f_l = \sum_{j_z=-j_+}^{j_+} f_{j_+,j_z}^{LLL} c_{j_z}$, where c_{j_z} is a complex coefficient. Because of the TR relation $f_{j_+,-j_z}^{LLL} = -f_{j_+,-j_z}^{LLL}j$, f_l can be expressed in terms of $l+1$ linearly independent basis as

$$f_l(x,y,z) = \sum_{m=0}^{l} f_{j_+=l+\frac{1}{2},j_z=m+\frac{1}{2}}^{LLL} q_m, \tag{6}$$

where $q_m = c_{m+\frac{1}{2}} - jc_{-m-\frac{1}{2}}$ is a quaternion constant. On the other hand, it can be calculated that the rank of the linearly independent l-th order quaternionic polynomials satisfying Eq. 4 is just $\binom{l+2}{2} - \binom{l+1}{2} = l+1$, thus f_{j_+,j_z}^{LLL}'s with $j_z \geq \frac{1}{2}$ are complete.

The topological nature of the 3D LL problem exhibits clearly in the gapless edge states. Inside the bulk, LL spectra are flat with respect to l. As l goes large, the classical orbital radius r_c approaches the boundary with the radius R_0. For example, for a LLL state, $r_c = \sqrt{2l}l_G$. As $l > l_c \approx \frac{1}{2}(R_0/l_G)^2$, the wavefunctions concentrate on the boundary and become surface states. Their spectra become $E(l) \approx l(l+1)\frac{\hbar^2}{2mR_0^2} - l\hbar\omega_0$. When the chemical potential μ lies inside the gap, it meets the surface states with the Fermi angular momentum denoted by l_f. The edge spectra can be linearized around l_f as $H_{bd} = (v_f/R_0)\vec{\sigma} \cdot \vec{L} - \mu$ with $v_f = (2l_f+1)\hbar/(2MR_0) - \omega R_0$. This is the Dirac equation defined on a sphere with the radius R_0. It can be expanded around $\vec{r} = R_0\hat{e}_r$ as $H_{bd} = \hbar v_f(\vec{k} \times \vec{\sigma}) \cdot \hat{e}_r - \mu$. Similar reasoning applies to other Landau levels which also give rise to Dirac spectra. Due to the lack of Bloch wave band structure, it remains a challenging problem to directly calculate the bulk topological index. Nevertheless, the $\mathbb{Z}_2$ structure manifests through the surface Dirac spectra. Since each fully occupied Landau level contributes one Dirac cone on the surface, the bulk is $\mathbb{Z}_2$-nontrivial if odd number of LLs are occupied.

The above scheme can be easily generalized to arbitrary dimensions by combining the N-D harmonic oscil-

lator potential and SO coupling. For example, in 4D, we have $H^{4D,LL} = \frac{p_{4D}^2}{2m} + \frac{1}{2}m\omega_0^2 r_{4D}^2 - \omega_0 \sum_{1 \leq a < b \leq 4} \Gamma^{ab} L_{ab}$, where $L_{ab} = r_a p_b - r_b p_a$ and the 4D spin operators are defined as $\Gamma^{ij} = -\frac{i}{2}[\sigma^i, \sigma^j]$, $\Gamma^{i4} = \pm\sigma^i$ with $1 \leq i < j \leq 3$. The $\pm$ signs of Γ^{i4} correspond to two complex conjugate irreducible fundamental spinor representations of $SO(4)$, and the $+$ sign will be taken below. The spectra of the positive helicity states are flat as $E_{+,n_r} = (2n_r + 2)\hbar\omega$. Following a similar method in 3D, we prove that the quaternionic version of the 4D LLL wavefunctions satisfy the full equation of Eq. 4. They form the complete basis for quaternionic left-analytic polynomials in 4D. For each l-th order, the rank can be calculated as $\binom{l+3}{3} - \binom{l+2}{3} = \frac{1}{2}(l+1)(l+2)$.

We consider the interaction effects in the LLLs. For simplicity, let us consider the 4D system and the short-range interactions. Fermions can develop spontaneous spin polarization to minimize the interaction energy in the LLL flat band. Without loss of generality, we assume that spin takes the eigenstate of $\Gamma^{12} = \Gamma^{34} = \sigma^3$ with the eigenvalue 1. The LLL wavefunctions satisfying this spin polarization can be expressed as $\Psi^{LLL,4D}_{m,n} = (x+iy)^m(z+iu)^n e^{-\frac{r_{4D}^2}{4l_G^2}} \otimes |\alpha\rangle$ with $|\alpha\rangle = (1,0)^T$. The 4D orbital angular momentum number for the orbital wavefunction is $l = m + n$ with $m \geq 0$ and $n \geq 0$. It is easy to check that $\Psi^{LLL,4D}_{m,n}$ is the eigenstate of $\sum_{ab} L_{ab}\Gamma^{ab}$ with the eigenvalue $(m+n)\hbar$. If all the $\Psi^{LLL,4D}_{m,n}$'s are filled with $0 \leq m < N_m$ and $0 \leq n < N_n$, we write down a Slater-determinant wavefunction as

$$\Psi(v_1, w_1; \cdots; v_N, w_N) = \det[v_i^\alpha w_i^\beta], \qquad (7)$$

where the coordinates of the i-th particle form two pairs of complex numbers abbreviated as $v_i = x_i + iy_i$ and $w_i = z_i + iu_i$; α, β and i satisfy $0 \leq \alpha < N_m$, $0 \leq \beta < N_n$, and $1 \leq i \leq N = N_m N_n$. Such a state has a 4D uniform density as $\rho = \frac{1}{4\pi^4 l_G^2}$. We can write down a Laughlin-like wavefunction as the k-th power of Eq. 7 whose filling relative to ρ should be $1/k^2$. For the 3D case, we also consider the spin polarized interacting wavefunctions. However, it corresponds to that fermions concentrate to the highest weight states in the equatorial plane perpendicular to the spin polarization, and thus reduces to the 2D Laughlin states. In both 3D and 4D cases, fermion spin polarizations are spontaneous, thus low energy spin waves should appear as low energy excitations. Due to the SO coupled nature, spin fluctuations couple to orbital motions, which leads to SO coupled excitations and will be studied in a later publication.

One possible experimental realization for the 3D LL system is the strained semiconductors. The strain tensor $\epsilon_{ab} = \frac{1}{2}(\partial_a u_b + \partial_b u_a)$ generates SO coupling as $H_{SO} = \hbar\alpha[(\epsilon_{xy}k_y - \epsilon_{xz}k_z)\sigma_x + (\epsilon_{zy}k_z - \epsilon_{xy}k_x)\sigma_y + (\epsilon_{zx}k_x - \epsilon_{yz}k_y)\sigma_z]$ where $\alpha = 8 \times 10^5$ m/s for GaAs. The 3D strain

configuration with $\vec{u} = \frac{f}{2}(yz, zx, xy)$ combined with a suitable scalar potential gives rise to Eq. 1 with the correspondence $\omega_0 = \frac{1}{2}\alpha f$. A similar method was proposed in Ref. [8] to realize 2D quantum spin Hall LLs. A LL gap of 1mK corresponds to a strain gradient of 1% over 60 μm, which is accessible in experiments. Another possible system is the ultra-cold atom system. For example, recently evidence of fractionally filled 2D LLs with bosons has been reported in rotating systems [51]. Furthermore, synthetic SO coupling generated through atom-light interactions has become a major research direction in ultra-cold atom system [52, 53]. The SO coupling term in the 3D LL Hamiltonian $\omega\vec{\sigma} \cdot \vec{L}$ is equivalent to the spin-dependent Coriolis forces from spin-dependent rotations, i.e., different spin eigenstates along $\pm x$, $\pm y$ and $\pm z$ axes feel angular velocities parallel to these axes, respectively. An experimental proposal to realize such an SO coupling has been designed and will be reported in a later publication [54].

In conclusion, we have generalized the flat LLs to 3D and 4D flat spaces, which are high dimensional topological insulators in the continuum without Bloch-wave band structures. The 3D and 4D LLL wavefunctions in the quaternionic version form the complete bases of the quaternionic analytic polynomials. Each filled LL contributes one helical Dirac Fermi surface on the open boundary. The spin polarized Laughlin-like wavefunction is constructed for the 4D case. Interaction effects and topological excitations inside the LLLs in high dimensions would be interesting for further investigation. In particular, we expect that the quaternionic analyticity would greatly facilitate this study.

Note Added: Near the completion of this manuscript, we learned that the 3D Landau level problem is also studied by S. C. Zhang [55].

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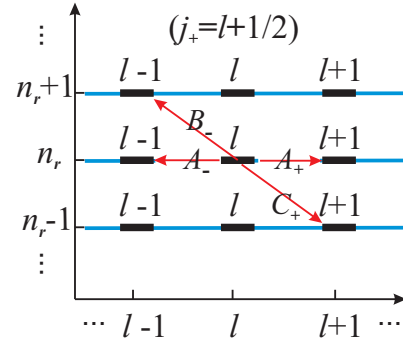[52] Y. J. Lin, K. Jiménez-García, and I. B. Spielman, Nature **471**, 83 (2011).

FIG. 2: The algebra structure of the 3D Landau levels in the positive helicity sector. Operators $A_{\pm}$ connect states with different l in the same Landau level, while B_- and C_+ connect those between neighboring Landau levels.

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Supplementary material for "Topological insulators with quaternionic analytic Landau levels"

In this supplementary material, we present several points including the ladder algebra to explain the degeneracy of the 3D Landau level (LL) wavefunctions, the quaternionic version of the 3D lowest Landau level (LLL) states with the negative helicity, the numerical calculation on the 3D LL spectra with the open boundary, and the generalization of LLs to an arbitrary dimension.

We have shown in the main text that there is no magnetic translation symmetry for 3D LL Hamiltonian. Nevertheless, the spectra flatness can still be understood by constructing the following ladder algebra structures. For example, we take the case of $qG > 0$ and consider the positive helicity Landau level states of H_+. The variable transformation for the radial eigenstates is applied as $\chi_{n_r,l}(r) = rR_{n_r,l}(r)$, and the corresponding radial Hamiltonians become

$$\hat{H}_l = \hbar\omega_0(-\frac{d^2}{dr^{*2}} + \frac{l(l+1)}{r^{*2}} - l + \frac{1}{4}r^{*2}), \quad (8)$$

where the dimensionless radius reads as $r^* = r/l_G$. The ladder operators are defined as

$$A_+(l) = \frac{d}{dr^*} - \frac{l+1}{r^*} - \frac{1}{2}r^*,$$
$$A_-(l) = -\frac{d}{dr^*} - \frac{l}{r^*} - \frac{1}{2}r^*. \quad (9)$$

They satisfy the relations $\hat{H}_{l\pm1}A_{\pm}(l) = A_{\pm}(l)\hat{H}_l$. Consequentially, $\chi_{n_r,l\pm1} = A_{\pm}(l)\chi_{n_r,l}$ with the same energy independent of l. All the states in the same LL can be
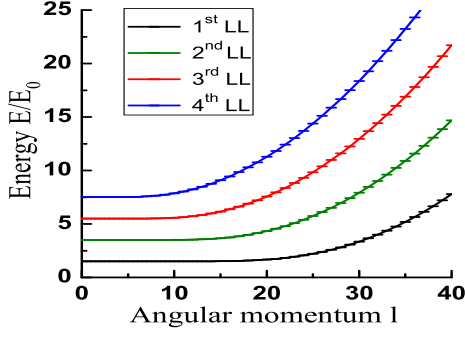
FIG. 3: The energy dispersion of the first four Landau levels *v.s.* $l = j - \frac{1}{2}$. Open boundary condition is used for a ball with the radius $R_0/l_G = 8$. The edge states correspond to those with large values of l and develop linear dispersions with l. The most probable radius of the LLL state with l is $r = l_G \sqrt{l}$.

reached by successively applying $A_\pm$ operators. To connect different LLs, other two ladder operators are defined as

$$B_-(l) = -\frac{d}{dr^*} - \frac{l}{r^*} + \frac{1}{2}r^*$$
$$C_+(l) = \frac{d}{dr^*} - \frac{l+1}{r^*} + \frac{1}{2}r^*, \qquad (10)$$

which satisfy $H_{l-1}B_-(l) = B_-(l)(H_l + 2\hbar\omega_0)$ and $H_{l+1}C_+(l) = C_+(l)(H_l - 2\hbar\omega_0)$, respectively. By applying $B_-(l)$ ($C_+(l)$) to $\chi_{n_r,l}(r)$, we arrive at $\chi_{n_r+1,l-1} = B_-(l)\chi_{n_r,l}$ and $\chi_{n_r-1,l+1} = C_+(l)\chi_{n_r,l}$ with the energy change $\pm 2\hbar\omega_0$, respectively, as illustrated in Fig. 2. Similar algebra can also be constructed for the case of $qG < 0$.

We have numerically calculated the spectra of the 3D LL Hamiltonian with the open boundary condition for the positive helicity states with $j_+ = l + \frac{1}{2}$. The results for the first four LLs are plotted in Fig. 3. The radius of the boundary is $R_0/l_G = 8$. For the lowest LL (LLL) states, when the orbital angular momentum l exceeds a characteristic value $l_c \approx 30$, the spectra become dispersive indicating the onset of surface states.

In the main text, we have showed that the 3D LLL states with the positive helicity in the quaternion representation form a set of complete basis for the quaternionic left-analytic polynomials. For the case of the LLL with negative helicity, their quaternionic version $g_{j_-,j_z}^{LLL}(x,y,z)$ are not analytic any more. Nevertheless, they are related to the analytic one through $g_{j_-=(l+1)-\frac{1}{2},j_z}^{LLL} = (-xk-yj+zi)f_{j_+=l+\frac{1}{2},j_z}^{LLL}i$.

The study in 3D and 4D LL systems can be generalized to N-D by replacing the vector and scalar potentials in Eq. 1 in the main text with the $SO(N)$ gauge field $A^a(\vec{r}) = gr^bS^{ab}$ and $V(r) = -\frac{N-2}{2}m\omega_0 r^2$, respectively, where S^{ab} are the $SO(N)$ spin operators constructed based on the Clifford algebra. The rank-k Clifford algebra contains $2k+1$ matrices with the dimension $2^k \times 2^k$ which anti-commute with each other denoted as Γ^a ($1 \leq a \leq 2k+1$). Their commutators generate $\Gamma^{ab} = -\frac{i}{2}[\Gamma^a, \Gamma^b]$ for $1 \leq a < b \leq 2k+1$.

For odd dimensions $N = 2k+1$, the $SO(N)$ spin operators in the fundamental spinor representation can be constructed by using the rank-k matrices as $S^{ab} = \frac{1}{2}\Gamma^{ab}$. For even dimensions $N = 2k+2$, we can select $2k+2$ ones among the $2k+3$ Γ-matrices of rank-$(k+1)$ to form $S^{ab} = \frac{1}{2}\Gamma^{ab}$, then all of S^{ab} commute with Γ^{2k+3}. This 2^{k+1}-D spinor Rep. of S^{ab} is thus reducible into the fundamental and anti-fundamental Reps. Both of them are 2^k-D, which can be constructed from the rank-k Γ-matrices as $S^{a,2k+2} = \pm\frac{1}{2}\Gamma^a(1 \leq a \leq 2k+1)$ and $S^{ab} = \frac{1}{2}\Gamma^{ab}(1 \leq a < b < 2k+1)$, respectively. As for TR properties, Γ^a's are TR even and odd at even and odd values of k, respectively. We conclude that at $N = 2k+1$, the N-D version of the LL Hamiltonian is TR invariant in the fundamental spinor Rep. At $N = 4k$, it is also TR invariant in both the fundamental and anti-fundamental representations. However $N = 4k+2$, each one of the fundamental and anti-fundamental Reps is not TR invariant, but transforms into each other under TR operation.

Similarly, the N-D LL Hamiltonian can be reorganized as the harmonic oscillator with SO coupling. For the case of $qG > 0$, it becomes

$$H_{N,+} = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 r^2 - \hbar\omega_0\Gamma_{ab}L_{ab}, \qquad (11)$$

where $L_{ab} = r_a p_b - r_b p_a$ with $1 \leq a < b \leq N$. The l-th order N-D spherical harmonic functions are eigenstates of $L^2 = L_{ab}L_{ab}$ with the eigenvalue of $\hbar^2 l(l+D-2)$. The N-D harmonic oscillator has the energy spectra of $E_{n_r,l} = (2n_r + l + N/2)\hbar\omega$. When coupling to the fundamental spinors, the l-th spherical harmonics split into the positive helicity (j_+) and negative helicity (j_-) sectors, whose eigenvalues of the $\Gamma_{ab}L_{ab}$ are $\hbar l$ and $-\hbar(l+N-2)$, respectively. For the positive helicity sector, its spectra become independent of l as $E_+ = (2n_r + N/2)\hbar\omega$, with the radial wave functions are

$$R_{n_r l}(r) = r^l e^{-r^2/4l_G^2} F(-n_r, l + N/2, r^2/2l_G^2). \qquad (12)$$

The highest weight states in the LLL can be written as

$$\psi_{ab,\pm l}^{hw}(\vec{r}) = [(\hat{e}_a \pm i\hat{e}_b) \cdot \vec{r}]^l e^{-r^2/4l_G^2} \otimes \alpha_{\pm,ab}, \qquad (13)$$

where $\alpha_{\pm,ab}$ is the eigenstate of Γ_{ab} with eigenvalue ± 1, respectively. The magnetic translation in the ab-plane by the displacement vector $\vec{\delta}$ takes the form $T_{ab}(\vec{\delta}) = \exp[-\vec{\delta} \cdot \vec{\nabla} + \frac{i}{2l_G^2}\Gamma_{ab}(r_a\delta_b - r_b\delta_a)]$. Similarly to the 3D case, staring from the LLL state localized around the origin with $l = 0$, we can perform the magnetic translation and Fourier transformation with respect to the transverse spin polarization. The resultant localized Gaussian pockets are LLL states of the eigenstates of the $SO(N-1)$ symmetry with respect to the translation direction $\vec{\delta}$. Again each LL contributes to one channel of surface Dirac modes on S^{N-1} described by $H_{bd} = (v_f/R_0)\Gamma_{ab}L_{ab} - \mu$.